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PHYSICAL IDEAS OF THE METHOD OF ELEMENTARY EXCITATIONS
(The Many-Electron Problem in the Theory of the Solid State)

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PHYSICAL IDEAS OF THE METHOD OF ELEMENTARY EXCITATIONS (The Many-Electron Problem in the Theory of the Solid State)

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ABSTRACT. The application of the many-electron theory of solids involving the behavior of a large number of interacting particles is proposed for the clarification of certain paradoxes and the solution of new problems in the theory of metals which the single electron is incapable of handling. The solution of the formulated problem is associated with severe difficulties due to complexity of the wave equation for the system of many ($\sim 10^{23}$) interacting particles and due to the necessity of computing complex statistical sums. The problem can be simplified substantially by considering only the weakly excited state of the system. The hypothesis of elementary excitation is examined in the light of recent developments in solid-state physics to show its physical implications and its scope of application in the solution of new problems associated with the solid state.

SECTION 1. INTRODUCTION. THE DIFFICULTIES ASSOCIATED WITH THE "SINGLE-ELECTRON" THEORY OF METALS.

The problem of investigating systems which consist of a large number of /55* interacting particles occupies one of the key places in the modern physics of condensed media. As we shall see, this problem is particularly acute in the theory of the metal state (as well as in the theory of the liquid); however, even in the theory of semiconductors, where it would seem that the interaction of conduction electrons can be neglected because their concentration is small, there are problems encountered in which it is absolutely necessary to take electron interaction into account. It is sufficient to recall the following common argument: as a result of (for example) nonuniform distribution of impurities in the lattice, the electron concentration in the lattice is also different at different points and the redistribution of electrons continues until the resulting space charge produces a field which inhibits a further mixing of electrons. Arguments of this type are constantly encountered in the theory of surface states, of photoelectromotive force, etc., and it is clear that such arguments have been based entirely on the presence of electron interaction. At the same time the correct solution of quantum mechanical (and also of the classical) problem on the behavior of a system consisting of a large number of interacting particles poses substantial difficulties. In the present article, without going into the details of calculations, we shall try to present the substance of one of the methods for the approximate solution of the problem of a large number of bodies, which appears to be most promising to us and which is being

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Numbers in the margin indicate pagination in the original foreign text.

developed in a most interesting manner at the present time. No claims are made to the completeness of the presentation; our problem is merely to acquaint /56 the non-theoretical reader with the substance of the matter.

Since the basic sphere of application for the methods of solving the problem of many bodies is currently the physics of solids, it is appropriate that we start our discussion by considering some of the difficulties associated with the modern theory of metals. This theory which has neglected the actual strong interaction between electrons and until the present day has been developed almost exclusively as a single-electron theory* in which the correlation between electrons was either completely ignored (the simplest model of an "electron gas" ref. 1), or which was taken into account very approximately by the method of the self-consistent field). Nevertheless, series of qualitative conclusions which follow from the "single-electron" theory (even in its most primitive form) are in good agreement with experiment. This includes, for example, the temperature dependence of electrical conductivity and the electron heat-capacity of metals, the theory of paramagnetism for alkaline metals, and others. At first glance this situation appears to be paradoxical; a physically unsound theory leads to correct results; obviously (ref. 2) the problem of the theory of metals first involves an understanding of the reasons for this paradox**. We note, however, that the successes of a "single-electron" model should not be overemphasized (nevertheless, this overemphasis in regard to the band theory of metals unquestionably exists in a series of works***); in this respect the books by Mott, Jones and Seitz referenced above are characteristic.

* An exception to this is only the theory of ferromagnetism, in which the necessity of an essentially "many-electron" formulation was long ago recognized.

** An effort to solve the problem in a trivial manner, by assuming that the electrons of interaction energy is small compared to the electron kinetic energy, has proven to be inconsistent. Indeed the Fermi energy for the electron gas, as we know, is given by the equation

$$E_F = (3\pi^2)^{2/3}\frac{\hbar^2}{2m}n^{2/3},$$

where n is the number of electrons per unit volume; m is the mass of the electron; while the average energy of Coloumb interaction is obviously of the order

$$e^2 n^{1/3}.$$

The ratio of these energies is of the order of $4\cdot 10^7 n^{-1/3}$, which for rational values of n (approximately 10^{22} cm^3) represents a quantity which is of the order of unity. As it appears to us, this situation destroys the very concept of the "Fermi Sphere" for electrons in a metal.

*** The band theory of metals has been frequently subjected to justifiable critism in the works of Soviet scientists (refs. 2-6).

A series of phenomena cannot at all be explained within the framework of a "single-electron" theory (such phenomena apparently include superconductivity), while other phenomena are explained only formally, so to speak. Probably the strongest example of such a formal explanation is encountered in the theory on the magnetic properties of metals at low temperatures. As we know, at low /57
temperatures the magnetic susceptibility of a series of metals depends in a periodic manner on the magnetic field intensity H. From the qualitative standpoint this effect appears to be explained very well by the "single electrons" theory (refs. 7-9), which provides for the necessary periodic relationship. When the parameters contained in the theoretical formula (for the effective mass* and the concentration of conduction electrons) are selected in a particular manner we also obtain a quantitative agreement between theory and experiment. However, a more careful examination of the problem (ref. 10) shows that this explanation is illusory to a large extent. Specifically, for the parameters contained in the theoretical equation, we find values which are unreasonably small (and which do not agree with data obtained from other measurements). Thus, for example, in the case in zinc, the number of conduction electrons corresponding to a single atom is found to be of the order of $0.8 \cdot 10^{-6}$ which, as shown in reference 11, represents only 1/1000 of the number necessary to explain the values of the electron heat capacity of this metal as observed experimentally. This situation is the same for other metals (beryllium and bismuth). Thus it turns out that the "single electron" theory gives only a correct qualitative nature of the relationship but not the quantitative side of the picture. However, the form of curve X(H) is determined to a large measure only by the statistical properties of the system. Only the numerical characteristics of the curve are associated with the specific values of the parameters which depend on the nature of the system (for example masses, charges and particle concentrations).

In view of this, we should point out that in order to obtain, for example, the qualitative picture of the variation in the electron heat capacity as a function of temperature, we must know only the statistics of electrons; similarly, only the statistical properties of electrons and of the thermal lattice oscillations determine the form of the temperature dependence for the electrical conductivity of metals.

Thus, in a single-electron theory not all the relationships are properly obtained, but rather only those which basically are due, to the statistical properties of the system--by the fact that the electrons satisfy the Fermi statistics. On the other hand, those laws which depend specifically on the form of the energy spectrum and on the specific values which determine its parameters are usually not conveyed by the "single electron" theory of metals.

In order to clarify the above "paradox" and also in regard to the investigation of problems in the theory of metals which have not been solved to date, /58

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It would be more correct to say "effective masses" because, due to the anisotropy of crystalline lattices in the metals considered, the electrons in these metals are characterized by three effective masses rather than by one effective mass (masses corresponding to the three principal axes of the crystal).

it becomes necessary to use a "many-electron" approach to the problem. Thus, we must turn to the problem concerning the investigation of the properties of a system consisting of a large number of particles which interact.

SECTION 2. THE HYPOTHESIS OF "ELEMENTARY EXCITATIONS"

The difficulties associated with the solution of the problem formulated are as follows:

a) the wave equation for a system consisting of a large number (approximately 10^{23}) of interacting particles is exceptionally complex; its exact solution is hardly possible by the methods of modern mathematics, even if a computer is used.

b) even if it were possible to determine the possible energy levels of the system considered with a large number of bodies, it would still be necessary to compute the following statistical sum to find a series of quantities which are observed experimentally (heat capacity, magnetic susceptibility, etc.):

$$Z=\sum_n e^{-\frac{E_n}{kT}} . \qquad (2.1)$$

(E_n are the possible energy levels numbered by the subscript n.) Indeed, if we know Z we can find the free energy and consequently all the thermodynamic properties of the system. Generally speaking, this problem is somewhat simpler than the first (we recall that the classical analogy (2.1) represents an interval with a multiplicity of approximately 10^{23}, where the expression under the integral sign, generally speaking, is not represented in the form of a product of co-factors each of which depends on a small number of variables).

The above difficulties are particularly serious and, considering the state of modern mathematics, it is hardly reasonable to try to solve them directly. However, by considering the expression for the statistical sum (2.1) it is clear that in practice this formulation of the problem is not mandatory. Indeed, a significant role in (2.1) is played only by the energy levels which are close to the basic one. Therefore, we can limit ourselves to the investigation of such "weak excitations" of the system's states. This situation, as we shall see, simplifies the problem tremendously.

In some specific cases the problem of the weakly excited states of a system consisting of a large number of particles has long been solved. In this connection we recall two well-known examples and consider them (from a purely qualitative point of view), remembering to expose certain special features associated with the behavior of such systems which, as will be shown later, are of a completely general nature.

A. Oscillations of a Crystalline Lattice

The problem of the thermal oscillations of a crystalline lattice apparently represents the first historic example involving the investigation of the collective behavior of a large number of interacting particles. Apparently, in this case the lowest energy state pertains to one of "complete orderliness" when all the atoms (or ions) of the lattice are uniformly (and periodically) distributed in space*. The excitation of the system consists of the origin of small oscillations of atoms near the position of equilibrium; in this case the spatial distribution of atoms will naturally be slightly heterogeneous. In other words, the excitation of the system in this case consists of the occurrence of certain "special states"--local variations in density; the latter are not "frozen" in a single place but rather propagate over the entire lattice as waves (a particular case of these waves are the conventional sound oscillations). /59

For small (compared with interatomic distances) amplitudes of oscillations (this is precisely the condition for "small excitation") the principle of superposition is valid for elastic waves, i.e., these waves propagate independently of one another and the energy of the system is the sum of the energies of the individual waves.

In the quantum mechanical consideration of the problem (refs. 12-14) these waves are naturally associated with discrete formations--sound quanta** (phonons). The interaction between the latter is absent as soon as the principle of superposition becomes valid for the respective waves ("harmonic" approximation).

Thus, from the energy point of view, the weakly excited state of a crystalline lattice may be looked upon as an "ideal gas" consisting of certain "quasi particles"--phonons. We should like to emphasize that these quasi particles have nothing in common with atoms which constitute the system in question but rather represent the corpuscular aspect of the collective oscillatory motion of the latter.

The state of the phonon (in a simple lattice) is determined by its polarization (longitudinal or transverse wave) and by three components of some vector (in many respects analogous to the impulse), which are used to establish the energy. Since the values of sound intensity in the lattice, possible in principle, are not limited***, any number of "quasi particles" may be in the same state; consequently they satisfy the Bose-Einstein statistics (irrespective of the type of statistics satisfied by the atoms making up the lattice). As we know, by using the concept of phonons we can construct the entire thermodynamics

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* Our arguments follow a purely "classical" approach and we neglect the existence of zero oscillations, whose presence is insiginificant for our discussions.

** The concept of sound quanta was first introduced by I. Ye. Tamm (ref. 12).

*** Of course, when the sound waves are of sufficiently strong intensity these

(Footnote continued on next page).

of a crystalline lattice and also examine a series of kinetic processes which take place in it.

B. Spin Waves in a Ferromagnetic Material

The second example which we wish to consider pertains to weakly excited states of ferromagnetic materials. As we know (ref. 15), the basic energy level of a ferromagnetic material corresponds to a state of "complete magnetization" when the magnetic moments of all the lattice atoms are oriented in the same manner* (the spins of all the "magnetic"** electrons have the same component along some axis).

The excitation of the system consists of a change in the direction of the magnetic moments of certain atoms (in the inversion of spins in part of the "magnetic" electrons), i.e., as in the first example, it consists of the occurrence of certain special states (in this case, of spins with the same direction in a "medium" of spins with opposite direction) which propagate as waves over the entire crystalline lattice.

Indeed, in view of the physical equivalence of various nodes of the lattice it is obvious that a state with "inverted spin" cannot "get stuck" in some one particular atoms***, but will propagate over the lattice due to the interaction of electrons. In the stationary state the inverted spin may be uncovered with the same probability in any atom of the lattice (if the lattice is a simple one). These states are called spin waves. As long as the number of inverted spins is small compared with the total number of "magnetic" electrons (conditions for the level of excitation) and, consequently, the probability of their encounter in the lattice is small, we may assume that the spin waves propagate independently of one another and each of them is characterized by a specific energy. In this case the energy of the system of electrons (with an accuracy /61
determined by an insignificant additive constant) is composed of the energies of individual spin waves. Naturally, the latter may be looked upon as certain "quasi particles" (sometimes called "ferromagnons" because they are characteristic of ferromagnetic materials), and as in the first example we arrive at a concept of an ideal gas consisting of "quasi particles" which represent a weakly excited state of a system of particles which undergo strong interactions (in this case electrons in a ferromagnetic material). We should like to

(Continued)

waves can no longer be looked upon as independent. This situation, however, is insignificant for our discussions (even because the corresponding intensities are much larger than those necessary to impart a Bose nature to the phonon statistics).

* If we take into account the weak magnetic interaction of electrons this proposition requires a certain refinement which, however, does not introduce any basic changes in our discussions.

** Magnetic electrons are those whose spins (in the absense of a magnetic field) are capable of orientation in any direction (i.e., for example, electrons contained in the unfilled atomic shells).

*** Here we are speaking only of an ideal lattice which does not contain any structural defects which would disrupt the translation invariance of the system.

emphasize again that these quasi particles have nothing in common with the electron* themselves but merely characterize the corpuscular aspect of their collective motion.

The concept of spin waves has proven very fruitful in the theory of ferromagnetism and has made it possible to establish theoretically the variation in the spontaneous magnetization close to saturation as a function temperature (ref. 16) and as a function of the external field (ref. 17) and has also made it possible to develop a quantum theory for magnetic anisotropy (ref. 18) and magnetostriction (ref. 19).

We can see that in both cases considered, the energy corresponding to the excited states of the system is represented as a sum of the energies of independent "quasi particles," and the investigation of the properties of the system in these states is reduced to the investigation of the quasi particle "gas" (i.e., to a problem which is well known and which can be solved without any difficulties). Because the systems which we have considered are entirely different physically, it is natural to assume that this proposition is characteristic of any quantum system consisting of a large number of interacting particles. The excitation of the system is always reduced to the occurrence of certain special states--"elementary excitations," which (in view of the translational invariance) propagate in a wave-like fashion over the system; the weakly excited states of any quantum system consisting of a large number of interacting particles may be represented as an ideal gas consisting of certain "quasi particles" which replace these waves**.

The possible values of the energy of the quasi particles, their moment of momentum and other similar quantities as well as the statistics by the elementary excitations characterize completely the weakly excited states of the system. (Depending on the statistics of the elementary excitations, we speak of the Fermi type or the Bose type spectra (ref. 14) and the terms "Fermi" and "Bose" branches are sometimes used.) The quasi particles about which we are speaking in general have nothing in common with those particles which constitute the given system but represent merely a specific feature of their collective motion***.

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In this connection we note the known fact that spin waves (ref. 15) satisfy the Bose statistics rather than the Fermi statistics, as in the case of electrons.

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As far as we know, this idea was first expressed by L. B. Landau. In recent years it has been the subject of investigation by N. N. Bogolyubov, S. B. Vonsovskiy and by a series of other Soviet scientists.

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It follows from what we said that, for example, it would be entirely meaningless to attempt to collect the quasi particles (for example phonons) into a "box." They exist only to the extent of the existence of a system of interacting particles which undergo collective motion reflected by the concept of quasi particles; when the system is destroyed (for example, when the crystal is vaporized) the corresponding elementary excitations naturally vanish.

It is quite obvious that the concept of elementary excitations immediately /62
solves both difficulties mentioned above in the theory of many bodies. Indeed, as soon as the values of the energy corresponding to the weakly excited state of the system are expressed in the form

$$E = \sum_k w(k)\, n(k), \tag{2.2}$$

where n(k) is the number of elementary excitations characterized by the set of "quantum numbers" k (for example by impulse, spin, etc.), the problem is reduced to the computation of the energy associated with a single quasi particle, w (k). We can expect that this will be much simpler than to solve the problem of a large number of bodies in its general formulation. Indeed, in a series of cases the energy spectrum of elementary excitations may be computed quite effectively. The different weakly excited levels of the system are obviously associated with various sets of numbers n(k), i.e., with different distributions of elementary excitations according to their quantum states.

Furthermore, the problem of computing the statistic sum in this case generally loses its acuteness because we are now dealing with an ideal gas for which the equilibrium function of particle distribution according to energy is well known.

Finally, it is clear that the concept of elementary excitations makes it possible to examine nonequilibrium problems without any special difficulty. Indeed, since definite values of energy are associated with the quasi particles and since the charge impulses, etc., may also have definite values, we can say that these transport their respective quantities. In this way, problems concerning transport processes in condensed media are reduced to analogous problems in the kinetic theory of an ideal gas. For example, the examination of heat conductivity, due to the lattice itself, is reduced to the study of energy transport by a flux of phonons. The problems concerning the establishment of statistical equilibrium in the system may also be examined by the method of elementary excitations without any special difficulty. In this case it is only necessary to introduce (as the next approximation) the weak interaction between quasi particles which leads to the establishment of equilibrium Fermi or Bose distribution by states. Indeed, from the point of view concerning the elementary excitations, the establishment of therodynamic equilibrium in a system with a large number of interacting particles is reduced to the establishment of the /63
equilibrium distribution of quasi particles in the gas.

The effectiveness of the method of elementary excitations has been demonstrated in a series of works devoted to the solution of specific equilibrium and nonequilibrium problems. Among these works we should mention, first of all, the theory of the superfluidity of helium II (ref. 20-24) first successfully developed by L. D. Landau exclusively on the basis of the concept on elementary excitations*. In the work of M. N. Bogolyubov (ref. 21), which gives a

*We do not consider these investigations here because there is a detailed survey on the subject in the literature and we refer the reader to this survey (ref. 65).

theoretical calculation of the spectrum of elementary excitations in a gas of Bose particles, weakly interacting on one another, these concepts have been substantiated for the microscopic case. An example of the successful application of the method of elementary excitations is the theory of heat conductivity in paramagentic dielectrics developed by I. Ya Pomeranchuk (ref. 25). These materials contain specific excitations associated with the presence of exchange interaction of electrons in the paramagnetic atoms. Specifically as in the case of a ferromagnetic material, the excited states of the system in this case may differ from the basic state by a different distribution of magnetic moments (the difference compared with the ferromagnetic case is that the basic state no longer corresponds to complete magnetization. It is difficult to indicate the exact distribution of magnetic moments in the basic state of a paramagnetic material when the external field is absent; for our purposes, however, it is sufficient to know that some particular distribution does exist). Naturally the deviation from the basic distribution of magnetic moments is not localized to individual atoms but is propagated in a wave-like fashion over the entire lattice due to the interaction of electrons. These elementary excitations are called magnons. (For weakly excited states, when the number of magnons is small compared with the total number of atoms in a lattice, the energy of their interaction may be neglected and consequently the excitation energy is the sum of the energies of the individual magnons.) The magnons (which apparently satisfy the Fermi statistics) interact with phonons, thereby affecting their mean free path, and also take part in the transport of heat. As shown in ref. 25, this leads to specific peculiarities in the variation of heat conductivity x as a function of temperature at low temperatures (the function x(T) is found to be nonmonotonic).

In addition to this, the method of elementary excitations was used with success in investigating the approximation to the state of equilibrium in ferromagnetic materials and in paramagnetic materials (refs. 26, 27). It has also /64
been used in efforts to construct a many-electron theory of metals and semiconductors which we shall discuss in the next section.

We know, finally, that in all of these cases a successive (even though approximate) consideration of the problem of many bodies naturally leads to the concept of elementary excitations. This is true in the theory of anti-ferromagnetism which has been solved on the basis of several generalized concepts concerning spin waves (refs. 28-31); weakly excited states of molecular crystals are capable of being described by means of concepts on excitons (refs. 32-35) --"quasi particles," whose motion characterizes the displacement of excitation energy (which, for example, is obtained from light) from one node of the lattice to another.

This concept concerning the exciton can naturally be extended to the case of any homopolar crystal. If one of the atoms of the lattice has obtained a certain excess energy in some manner or other, it is clear that this energy will be transmitted to other atoms as a result of interatomic interaction (in the end this energy will be uniformly, on the average, distributed among them). The wave-like displacement of the excited state may be looked upon as the motion of the quasi—particle of the excitons*.

*The concept concerning the exciton in a somewhat different form may be extended
(Footnote continued on the next page).

Finally, the concept concerning elementary excitations is in fact widely used in the ordinary theory of semiconductors (see, for example, ref. 36). Indeed, the "holes" in semiconductors represent typical quasi particles describing those states in which there is an incomplete set of electrons in certain atoms (this example illustrates particularly well both an essentially "collective" nature of elementary excitation as well as the correspondence of this concept to physical reality). (Indeed it is doubtful that any one will deny the existence of "holes" in semiconductors, just as noboby would decide to attempt to collect them in some vessel.)

Now returning to the consideration of the above difficulties associated with the theory of metals it is easy to see that in principle they are immediately solved by the idea of elementary excitations. Indeed, from this point of view the known success of the "single-electron" model is entirely understandable: the system of many interacting electrons in the metal, like any system of a large number of interacting particles, is characterized by certain excitations and what has been called the electron in the Somerfield and Bloch theories is in fact not an electron but a "quasi particle": the "electron gas" in the primitive theory of metals is in fact a "gas of elementary excitations" of a many electron system satisfying the Fermi statistics. In /65
this sense we can say that in the theory of metals people have always used the language of elementary excitations without knowing it. Therefore, it is not strange that the laws which are explained basically only by statistics are correctly passed on by the (single-electron) theory (they are simply unrelated to its simplifying assumptions): it is equally clear why the "single electron" model meets with failure in the analysis of those characteristics of the system which require more specific information concerning its energy spectrum for the analysis*.

It should be emphasized that what we have presented should not be interpreted in any way as the final solution of difficulties associated with the modern theory of metals. Here we have indicated a possible path for the solution which, as it appears to us, is correct and promising but yet untraveled. Before we can consider the solution of the problem presented above to be satisfactory we must first prove that the energy of a system of electrons in a metal is indeed expressed in the form (2.2) and we must determine the form of the function $w(k)$ as well as the statistics of elementary excitations**.

to the case of ionic crystals. The examination of this question, however, is beyond the scope of our problem.

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It is clear from what we have said how fruitless are the efforts to quantitatively refine and improve the methods of the "single electron" theory which are still being undertaken in some works. It is true that these efforts are quite "harmless," because they do not distort the Fermi nature of the spectrum, but they are also useless to the same degree.

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In the future we shall see that, as a rule, the spectrum is mixed, i.e., there are excitations of both the Fermi type and the Bose type.

As a result of this it should be possible to clarify which particular excitations are possible in the particular system (it is obvious that in the given specific system not all types of elementary excitations are possible). For example, spin waves occur in ferromagnetic materials but not in a metal of the beryllium type where they are apparently absent. In other words, the question arises as to the development for methods for the investigation of the spectra of elementary excitations. We should like to emphasize the importance of this problem. The fact is that the simplicity of operations with elementary excitations (as long as their statistics are known in the form of the function w(k)) may easily send us on a wrong path of "adjusting" a particular excitation spectrum to suit experimental data without the necessary theoretical basis. This would create a certain apparent understanding and explanation of phenomena with the actual absence of both and the concept concerning elementary excitations would lose its meaning and interest***.

SECTION 3. ELEMENTARY EXCITATIONS AND THE ELECTRON THEORY OF SOLIDS

As we have seen in the preceding section, a series of difficulties associated with the electron theory of metals could in all probability be solved if we were able to represent the energy of weakly excited states of many-electron system as a set of elementary excitations. We should only bear in mind that in materials which exhibit metallic properties, at least some, (if not all) excitations must be characterized by two peculiarities:

a) their movement in the lattice must be accompanied by charge transport (otherwise they will not serve as current carriers),

b) there must be no consumption of finite energy for their formation.

Indeed in the contrary case, at low temperatures, the number of elementary excitations of a given type (i.e., the number of current carriers) would drop exponentially with a decrease in temperature. This would lead to a corresponding behavior in the electrical conductivity. Apparently this does not take place (it is true of course that the experimental question concerning the variation in the electrical conductivity of metals at low temperatures as a function of temperature is not quite clear to date). Also, in our opinion the elementary excitations of a many-electron system are specifically characteristic

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This statement should not be misinterpreted. Of course, we do not protest against the establishment, for example, of the effective mass of a wuasi particle from experimental data as long as it is shown that the excitation of a particular type can indeed occur in a given system. We should recognize, to the same degree, the rather important "inverse problem" of the theory of elementary excitations--the determination of the spectrum form from experimental data (rather substantial results in this direction have been obtained by I. N. Lifshits and his co-workers (refs. 66,67)). We merely wish to guard against possible efforts to simply postulate the existence of a particular spectrum without first investigating whether its occurrence is actually possible. We should point out that in all the works referenced above such an "adjustment" did not take place; the form of elementary excitations was established either on the basis of direct computation or by means of theoretical considerations of a qualitative nature.

of the metal state of a material and must satisfy the Fermi statistics*. Indeed, it is known from experiment that the heat capacity of a metal is a linear /67
function of the temperature. This relationship is easily obtained theoretically if the elementary excitations of a many-electron system form a degenerate Fermi gas; in the case of the Bose-type excitation usch a relationship may take place only under specific assumptions concerning the density of the energy levels. Indeed, the total energy E of the gas consisting of elementary excitations is given by the well-known relationship**.

$$E = \int_{\varepsilon_{\min}}^{\infty} \frac{\rho(\varepsilon)\, d\varepsilon}{\exp\left\{\frac{\varepsilon - \mu}{kT}\right\} \pm 1}, \qquad (3.1)$$

where μ is the chemical potential, ε is the energy of a specific excitation, $\rho(\varepsilon)d\varepsilon$ is the number of states in the energy interval $(\varepsilon, \varepsilon+d\varepsilon)$, the signs "+", "-" correspond to the Fermi and Bose statistics respectively.

For the degenerate Fermi-gas $\mu>0$ and $\frac{\mu}{kT} \gg 1$; as we know the asymptotic expansion in kT/μ yields (see, for example, ref. 14);

$$E \approx \int_{\varepsilon_{\min}}^{\mu} \varepsilon\rho(\varepsilon)\, d\varepsilon + \frac{\pi^2}{6}(kT)^2 \left\{\rho(\mu) + \mu \frac{\partial\rho(\varepsilon)}{\partial\varepsilon}\Big|_{\varepsilon=\mu}\right\}, \qquad (3.2)$$

which gives as a linear temperature variation in the heat capacity for any form of $\rho(\varepsilon)$.

On the other hand, as we know (ref. 14), for a gas which satisfies the Bose statistics, the chemical potential is always negative (and small in absolute value if the gas is degenerate); therefore, the expansion of type (3.2) does not take place, and the variation in E as a function of T is established by the specific form of the function $\rho(\varepsilon)$***.

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This does not mean that there is no Bose excitation branch in metal. Unquestionably this branch exists (at least in certain metals). We merely wish to state that apparently the Fermi branch of the energy spectrum must be present.

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If several types of excitations are present it is necessary to take a sum of expressions of type (3.1). When the values of ε are very large the very concept of elementary excitations becomes inaccurate; however, this region contributes practically nothing to the integral.

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In this case $\rho(\varepsilon)$ usually turned out to be such that the heat capacity is proportional to a higher power of temperature than the first and therefore is very small at low temperatures. Thus, for example, in the case of phonons in a simple lattice the heat capacity, as we know, turns out proportional to T^3.

In the present section we propose, without considering the computational side of the problem, to consider the modern state of the question concerning elementary excitations of a many electron system in metals and semiconductors.

Certain types of excitations are already known to us. These are the excitions and spin waves considered in the preceding section. It is clear, however, that by no means are they characteristic of a metal. Indeed, the exciton represents a neutral formation whose origin also requires a finite energy. Consequently, it is unrelated to the most characteristic property of metals--high electrical conductivity. In the same way, when we have a simple displacement of a state with an inverted spin (the spin wave) the electric charge is by no means displaced along the lattice* since the average number of electrons for each individual atom remains unchanged (ref. 37, 38). /68

Thus, the model of spin waves considered eariler (sometimes known as the "exchange model" (ref. 15)) actually describes a ferromagnetic dielectric rather than a metal. This is understandable because in the "exchange" theory of spin waves a very important feature of the metallic state has not been taken into account. This feature involves the collectivization of part of the electrons over all atoms of the lattice (it is precisely due to this process that the electrons acquire the capacity to move freely along the lattice and to form what are known as "free charges" in the phenomenological theory of electricity). In order that it be possible for us to use the theory of spin waves in the investigation of ferromagnetic metals it is necessary to generalize it somewhat, taking into account the inevitable collectivization of at least part of the electrons over all of the metal atoms. A generalization of this type was carried out in two directions. First of all we should bear in mind that in real metal ferromagnetism is apparently due to the electrons in the d-shells which are not completely filled; on the other hand, in electrical conductivity the principle role is apparently played by "peripheral" electrons which (before the formation of the crystalline metal lattice) belong to external atomic shells, and these are collectivized over all of the metal atoms. S. V. Vonsovskiy (refs. 39, 40) proposed that the d-electrons should be considered on the basis of a many-electron exchange model taking into account, additionally, their exchange interaction with collectivized electrons; the interaction of the latter, however, is not taken into account. Thus the energy spectrum of the entire system consists of two "branches"--a set of spin waves (excitations of the Bose type) and the sum of the energies of external electrons (they may be looked upon as excitations of the Fermi type). The presence of interaction between internal and external electrons is exhibited independence of the effective mass of the latter on the total spin of the first, i.e., on the magnetization of the specimen.

In the "s - d-exchange" model of this type** there is a simultaneous reflection of both ferromagnetic and electrical properties and (because we take into account the exchange interaction between internal and external electrons) it is possible to investigate their interrelation. It is obvious, however, /69

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See, however, the footnote on page 14.

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This name is associated with the fact that the external electrons are assumed to be initially (before the formation of the metal) in the s-states.

that the s—d-model does not completely solve the problem of determining the energy spectrum of a system of electrons in a metal because there is no basis for neglecting the interaction of "collectivized" electrons with one another (this fact is also mentioned in references 39 and 40). Also, the very possibility of dividing a single system of electrons into two "parts" ("internal" and "external" electrons) is by no means obvious; apparently in a more exact theory it will be necessary to do without such concepts, which represent excessive simulation.

In regard to the necessity of taking into account electron interaction, the second possible generalization of the theory of spin waves in more consistent. This generalization uses the so-called "polar" model (refs. 3, 4, 5, 28, 38, 41 and 42). According to this model the electrons in the basic state of the metal are uniformly distributed, on the average, over all of the atoms; the excitation of the system consists of the deviation in the distribution of the charge from the uniform state (more precisely from the periodic state), i.e., using more descriptive language, it consists of the transition of part of the electrons to foreign atoms, which generates an equal number of atoms in the lattice with an excess and deficiency of electrons (the corresponding states of the atoms are called polar, and the name of the model itself is associated with this fact). It is natural that due to the translational invariance of the system the polar states in an ideal crystal are not localized to specific atoms but can occur at any point in the lattice with equal probability. If we translate this to the language of elementary excitations, the polar states correspond to the quasi particles' "pairs" and "holes" --and the motion of these characterizes respectively the wave-like propagation of states with "super complete" and with deficient electrons*. It is obvious that the transport of electrical current is associated with the displacement of the pair or of the hole. The statistic satisfied by excitations of this type may be both a Fermi and a Bose one. Thus, for example, if in the normal state there is an odd number of electrons in the valance shell of the atom and if the super complete electron also occurs in the valance shell, then the pairs and the holes are associated with an integral spin and consequently satisfy the Bose statistics. On the other hand, it is possible to have a situation where the atoms in the basic state have an integral spin; then the spins of the pairs in the holes have half-integral values and satisfy the Fermi statistics. The first case was considered in the works S. V. Vonsovskiy referenced above, the second (using the beryllium type metal as an example) was briefly discussed in a work by the author (ref. 43).

The polar model was used in references 44 and 45 to investigate the electrical conductivity of metal and of its magnetic properties. In line with the /70
basic ideas associated with the method of elementary excitations, the problem in both cases was reduced to the investigation of the corresponding properties of an ideal gas of quasi particles--of pairs and holes. The statistic which was satisfied by the elementary excitations in reference 45 was not established. Reference 44 was concerned with excitations of the Bose type. This situation led to a special relationship for the variation in the electrical conductivity ρ as

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In the version of the polar model proposed by N. N. Bogolyubov and S. V. Tyablykov which is more complete mathematically, the terms "pairs" as well as "holes" are not introduced explicitly but the consideration of polar states leads to a situation so that the spin waves becomes associated with electrical charge transport.

as a function of temperature ($\rho=\frac{\gamma}{T}+\frac{\beta}{T^2}$, where γ and β are constants), and it is apparent that such a relationship is observed experimentally at low temperatures in such metals as cesium and others. It is signifciant that it cannot be obtained in any manner within the framework of a single-electron theory of metals (ref. 1) because the key role here is played precisely by the type of statistic which is satisfied by the current carriers (in the single-electron theory the current carriers are free electrons and the Fermi statistics for them lead to the well-known law: $\rho \sim T^{-5}$).

Reference 46 investigated the electrical conductivity of a metal within the framework of a slightly different version of the polar model: it was assumed that in the basic state the distribution of electron density has a maximum heterogeneity (almost all of the lattice nodes are occupied either by pairs or by holes), and the excitation of the system is associated with a decrease in the heterogeneity of charge distribution (a partial "depolarization" of the crystal), i.e., with a decrease in the number of pairs and holes. The corresponding elementary excitations also satisfy the Bose statistics and the temperature variation of electrical conductivity turns out to be the same as in reference 45. Essentially, in reference 46, the metal is looked upon as something resembling an ionic crystal. We are not convinced that this approach to the problem is sound (it is not very clear, for example, what will happen to the diffraction of X-rays); however, the methodological value of this cited work is not questioned.

The known success achieved by the polar model should not, however, conceal its serious defects, which are organically associated with its initial assumptions. It is clear from what has been said that in its modern form the polar model cannot be applied without a contradiction to "good" metals containing a large number of current carriers. Indeed, the occurrence of current carriers in the polar model is necessarily associated with the excitation of the system (the current carriers are absent in the basic state). Consequently, in weakly excited states (and it is only in this case that the method of quasi particles is applicable) there will be few current carriers and we shall obtain a substance with poor conductivity.

Moroever, in a series of cases it is necessary to have finite energy for the formation of pairs and holes, which should lead to an exponential relationship between electrical conductivity and other quantities as a function of temperature. Finally, it is not very clear what happens to the electron heat capacity of the metal in the polar model (with the Bose-type spectrum). We encounter analogous difficulties when we further generalize the polar model to the so-called polar-exciton model (ref. 5) which considers the simultaneous presence of three types of elementary excitations--pairs, holes and excitons. /71

One gets the impression that, generally speaking, in its modern form the polar-exciton model of a solid body describes a semiconductor with an atomic lattice rather than a metal. Indeed, it is precisely in the case of the semiconductor that we have an exponential variation in the number of current carriers as a function of temperature. In this connection we note that the

polar exciton model of a crystal was the one actually used to investigate the magnetic (ref. 47) and electric (ref. 48) properties of semiconductors. The latter work was the first to give a many-electron explanation for a series of propositions from the "conventional" (based on the single electron-approximation) theory of semiconductors. Specifically, an atomic crystal was considered in which the pairs and holes of the polar model satisfy the Bose statistics. It was shown that behavior of these excitations depends on what we expect from the "conventional" conduction electrons and holes from the theory of semiconductors (the energy spectrum is of the band type, finite energy is required to produce excitation, etc). However, the basic nature (which in some cases has practical significance), bears a difference in the types of statistics which is satisfied by the current carriers in line with the single- and many-electron theories. In the region of degeneration this situation will naturally lead to a sharp difference in predictions concerning the electrical and magnetic properties of semiconductors. The corresponding experimental investigations would be of substantial interest to the theory of solids. However, we should bear in mind that in semiconductors of the germanium or silicon type the spectrum of pairs and holes for the polar model is of the Fermi type. This case was considered in reference 68. As was to be expected, it turned out that in a semiconductor of this type the pairs behave analogously to the conduction electrons of the single-electron theory, which serves as a basis for the qualitative deductions from the latter (this refers both to an ideal lattice and also to a lattice with defects; to a certain degree this is also valid when external electric and magnetic fields are present). We note, however, that this substantiation by no means relates to the computation methods of the single-electron theory. All of the constants which characterize the form of the energy spectrum (the width of the forbidden zone, effective mass, etc.,) are computed in an entirely different manner in the many electron theory compared with the single-electron theory. Substantiation refers only to the qualitative concepts of these band models (which, incidentally, are of basic interest to the experimenter). /72

It does not follow from what has been said that we should completely give up the concepts of the polar model of a metal and limit its application to semiconductors. Apparently, excitations of the types considered above still exist in metals but do not exhaust the entire energy spectrum of the latter*. These excitations collectively form what can be called the "semiconductors" spectrum of a metal. They are equally possible in nonmetallic crystals and represent the general feature which is contained in the electron energy spectrum of all crystals with atomic lattices.

In metals, however**, there are apparently excitations of another type which do not require finite energy for their formation and which therefore are present even at low temperatures. (Apparently they satisfy the Fermi statistic.)

*In connection with this we should note that the methods proposed to date for computing the spectra of elementary excitations, in practice, do not provide a complete system of eigenfunctions of the Hamiltonian for the many-electron problem.

**It would be more correct to say that precisely those substances which contain specific excitations are metals.

The question of investigating this specific metallic branch of the energy spectrum remains open to date (very great mathematical difficulties are encountered in this problem). In this connection it becomes of interest to study even the simplest cases of spectra of this type--Fermi and those without an energy gap, where the current carriers must already exist in the basic state of the system. Apparently, the easiest system which can be considered is one of weakly interacting conduction electrons in the crystal. In this case, in order to determine the energy spectrum we can use the theory of perturbations (the small parameter is the one defining the ratio of conduction electron concentration to the number of nodes in a lattice per unit volume)*. The corresponding methodology was developed in reference 49 and used to compute the electron conductivity in metals according to the many-electron model in references 50 and 51. In the latter two works it has been shown that, as was to be expected, the "statistical" results produced by the single-electron theory (the temperature law of electrical conductivity) also remain valid when the current carriers are elementary excitations of the Fermi type. However, we should remember that the quantitative results (ref. 49) (and consequently ref. 50) are of limited meaning and in our opinion cannot be applied to real metals in which the concentration of conduction electrons is by no means small. It would be more accurate to consider these results as applying to semiconductors, where the conditions for the applicability of this method of computation are indeed satisfied.

Recently the representation of local density variations as elementary excitations of the many-electron system has received rather extensive development from a slightly different point of view (refs. 52-59) than the conventional polar model. In these works** the idea expressed long ago by Bloch (ref. 60) was developed in detail. According to this idea the elementary excitations of a many-electron system are nothing more than the propagation of sound waves in this system (i.e., deviations from the spatial homogeneous distribution of electrons--of the plasma oscillations type (ref. 61-62)). The corresponding "quasi particles"--phonons--naturally satisfy the Bose statistics***.

In reference 53 and particularly reference 57, however, it is shown that for the three-dimensional case, which is of real physical interest, the sound oscillations do not exhaust all the excitations of a many-electron system.

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This formulation of the problem is quite natural for the nondegenerate (or weakly degenerate) case. When strong degeneracy is present the role of the small parameter may be placed by the ratio of the average interaction energy to the Fermi energy (see ref. 68).

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In line with the basic arrangement of this article we concern ourselves only with the physical contents of these works without entering into a comparative evaluation of the computation methods developed in them. We merely wish to state that in our opinion the most complete and rigid consideration of the problem is given in reference 57.

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These concepts are rather similar to the polar model. Actually, however, the fluctuations of density to date have been investigated either by a method which does not exhibit excitations of the Fermi type or by neglecting the periodical
(Footnote continued on next page).

In addition to these, there is a Fermi branch of the spectrum, which apparently is of particular interest for our purposes. It is also significant that, unlike ordinary sound waves which propagate in neutral uncharge systems, the excitation of plasma oscillations requires an expenditure of finite energy E_0, and the value of this energy is by no means small: $E_0 = \hbar \sqrt{\frac{4\pi}{m} ne^2}$, where n is the number of electrons per unit volume, and m and e are the mass and the charge of the electron, respectively. When n is approximately equal to 10^{22} cm^{-3}, E_0 turns out to be approximately equal to 8.6 electron volts; therefore, at ordinary temperatures the plasma phonons are practically absent. Only /74 zero oscillations of the plasma are present. Precisely these as well as the Fermi branch are of interest to the theory of metals per se.

We note, however, that the study of plasma phonons may play a significant role in the retardation of fast charge particles moving through the metal* (the energy of the particle may be used to excite plasma oscillations). The investigation of the Fermi branch in this method of computation has not been carried out to date with the required degree of accuracy. In our opinion it is necessary that we take into account the atomic structure of the crystal, in particular the periodic field of the lattice (apparently this does not produce a noticable effect on plasma oscillations, or else the wavelengths in question are sufficiently large so that the discrete structure of the crystal is smeared).

In summarizing everything that has been said, we should acknowledge that at the present time the concept of elementary excitations (which started to develop only rather recently) has already produced important achievements and has permanently won its rightful place in the physics of condensed systems. In the application to the theory of the solids it may be assumed without dispute that the energy spectrum of a system of a large number of interacting electrons in the crystal has a "mixed" nature--it contains both a Bose branch as well as a Fermi branch. We may assume that the first one has been studied to a certain degree; apparently it is exhausted by the study of spin waves, (in ferromagnetic materials), excitons and fluctuations of the electron density (in some form or other).

(Footnote continued)
nature of the field in the crystalline lattice (the positive charge of this system was assumed to be equally distributed in space and its role consisted only in compensating for the total negative charge of the electrons). On the other hand the polar model in its modern form is significantly associated with the proposition on the correct periodic distribution of atoms in the crystalline lattice. It is possible that in the future, by generalizing the results of reference 57 to the case where a periodic field is present in the lattice, the polar model and the method of density fluctuations may turn out to be equivalent to some degree and will represent two different approaches to the same problem.

* In this connection also see references 63 and 64.

In regard to the second branch, at the present time it is only possible to investigate its "semiconductor" part. The creation of new computation methods which would make it possible to theoretically study the excitation of the "metallic" type appears to us to be one of the most urgent problems of the physics of solids.

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